Algorithm Theoretical Basis Document for the Northern High Latitude L3 Sea and Sea Ice Surface Temperature Chain

OSI-203-b
Version 1.3

STEINAR EASTWOOD (MET), GORM DYBKJÆR (DMI), CRISTINA LUIS (MET) AND JACOB HØYER (DMI)

NORWEGIAN METEOROLOGICAL INSTITUTE AND DANISH METEOROLOGICAL INSTITUTE

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1 Introduction

1.1 Scope

This algorithm theoretical basis document (ATBD) presents the Northern High Latitude (NHL) Level 3 Sea and Sea Ice Surface Temperature (SST/IST) product from the EUMETSAT Ocean and Sea Ice Satellite Application Facility (OSI SAF). The focus of the document is to present an overview of the algorithm and technical details of the proposed processing chain. It does not deal with aspects of user interface or present validation results, as those issues will be dealt with in subsequent and Product User Manual (PUM) and Validation Report (VR) .

1.2 Overview

The EUMETSAT OSI SAF produces a range of operational air-sea interface products, namely: wind, sea ice characteristics, Sea Surface Temperatures and radiative fluxes, Surface Solar Irradiance (SSI) and Downward Longwave Irradiance (DLI). More details on the products and OSI SAF project are available at http://www.osi-saf.org.

SST, IST, SSI and DLI products from the OSI SAF are produced using geostationary and polar orbiting satellites and are available in level 2 and level 3 formats, with different timeliness depending on the production setup.

A specific L3 Atlantic High Latitude SST/IST product (OSI-203-a) is produced at MET Norway covering the Northern High Latitudes north of 50N. This product is now extended with SST and IST from the OSI SAF L2 SST/IST product based on NPP VIIRS data (OSI-205-b), which this ATBD describes.

1.3 Scientific motivation

The L3 Sea and Sea Ice Surface Temperature product (OSI-203-b) is based on the development and operational history of the OSI-203 product that goes back to the beginning of the OSI SAF project (1997). Based on radiometric data from the AVHRR instruments, the OSI SAF team has worked with commonly used algorithms such as multichannel SST (McClain et al., 1985) and Nonlinear SST (Walton et al., 1998), with Nonlinear SST as the final choice. Since the OSI-203-b is a regional product, a motivation has been to use regional versions of the algorithm. Work including radiative transfer modelling both over open sea and sea ice has provided this and is further discussed in [RD.1].

The motivation for this upgrade is the inclusion of sea ice surface temperature in the product, as well as extending the product to cover high latitude areas over the whole Northern Hemisphere.

1.4 Glossary

Acronym	Description
ATBD	Algorithm Theoretical Basis Document
AVHRR	Advanced Very High Resolution Radiometer
CMS	Centre de Méteorologie Spatiale
DLI	Downward Longwave Irradiance
DMI	Danish Meteorological Institute
GHRSST	Group for High Resolution Sea Surface Temperature
HL	High Latitudes
HIRLAM	High Resolution Limited Area Model
IST	Sea Ice Surface Temperature
LML	Low and Mid Latitudes
MDS	Matchup Dataset
METNO	Norwegian Meteorological Institute
MIZ	Marginal Ice Zone
MSG	Advanced Very High Resolution Radiometer
NOAA	National Oceanic and Atmospheric Administration
NHL	Northern High Latitude
NPP	National Polar orbiting Partnership
NWC	Nowcasting
OSI SAF	Ocean and Sea Ice Satellite Application Facility
SSES	Sensor Specific Error Estimates
SSI	Surface Solar Irradiance
SST	Sea Surface Temperature
VIIRS	Visible Infrared Imaging Radiometer Suite

1.5 Applicable documents

[RD.1] Algorithm Theoretical Basis Document for the OSI SAF Sea and Ice Surface Temperature product OSI-205-b, v1.2.
[RD.2] HL SST matchup database format, v1.1.
[RD.3] OSI SAF Product Requirement Document, v3.3.
[RD.4] Product User Manual for the OSI SAF sea ice edge and type products (OSI-402 and 403), v1.2.

2 SST/IST processing scheme overview

This chapter gives an overview of the processing scheme used for processing the 12-hourly SST and IST product.

2.1 Product

The delivered products are 12-hourly means centred on 0 UTC and 12 UTC. The NHL product is derived from AVHRR data from the EUMETSAT METOP satellites. A combination of locally received data and data received through the EARS distribution system is used. The area to be covered is shown in Figure 1.

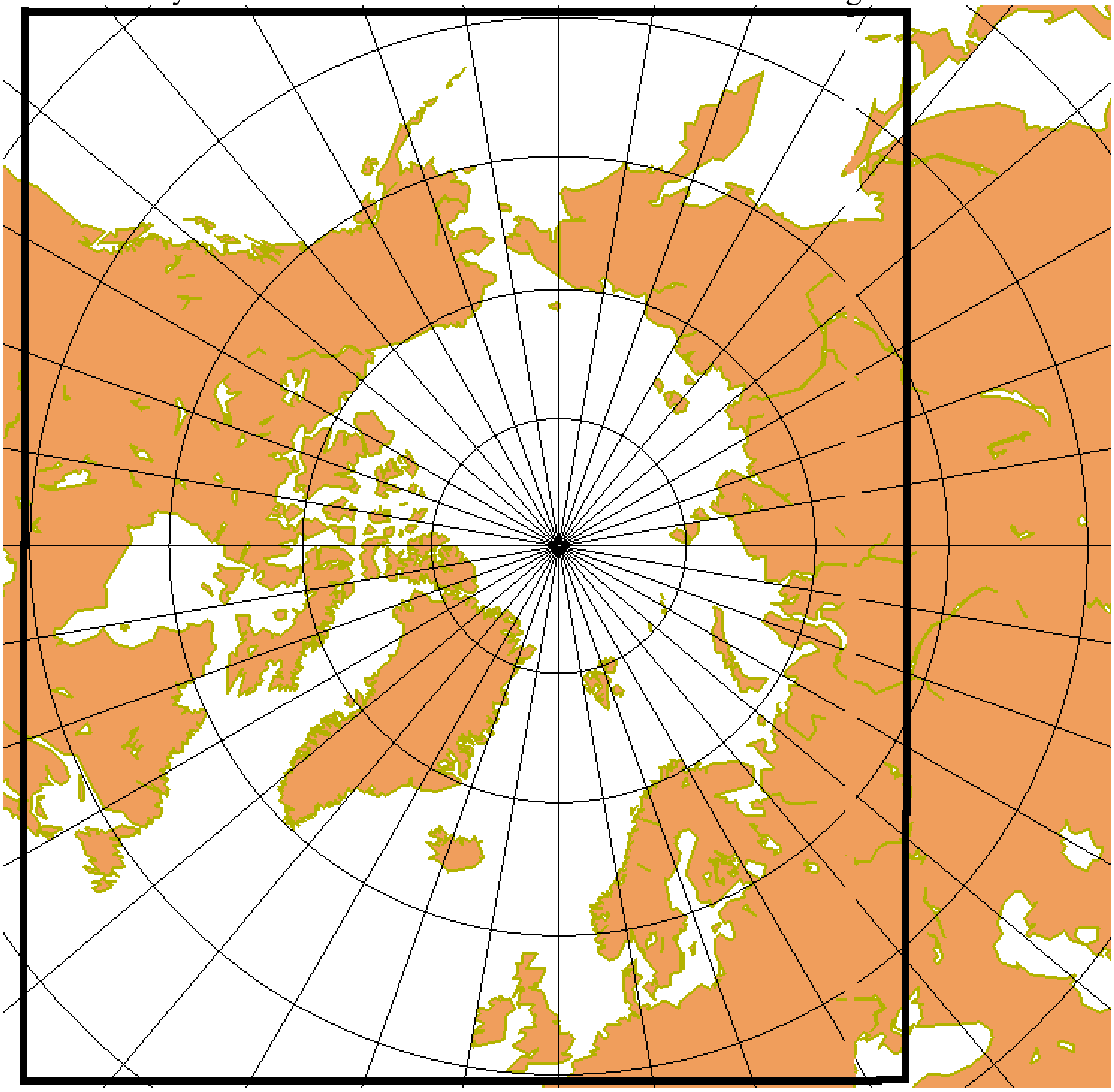

Figure 1: Coverage of NHL OSI SAF 12-hourly SST and IST product (marked by the black rectangle).

2.2 L2 satellite orbit processing chain

The input to the 12-hourly SST and IST processing is the L2 satellite orbit SST and IST product, OSI-205-b. The OSI-205-b is delivered both from AVHRR data from the METOP-A satellite and from NPP VIIRS data. The main L2 processing steps are shown on the left part of Figure 2. All details of the L2 processing is described in the OSI-205-b ATBD [RD.1] .

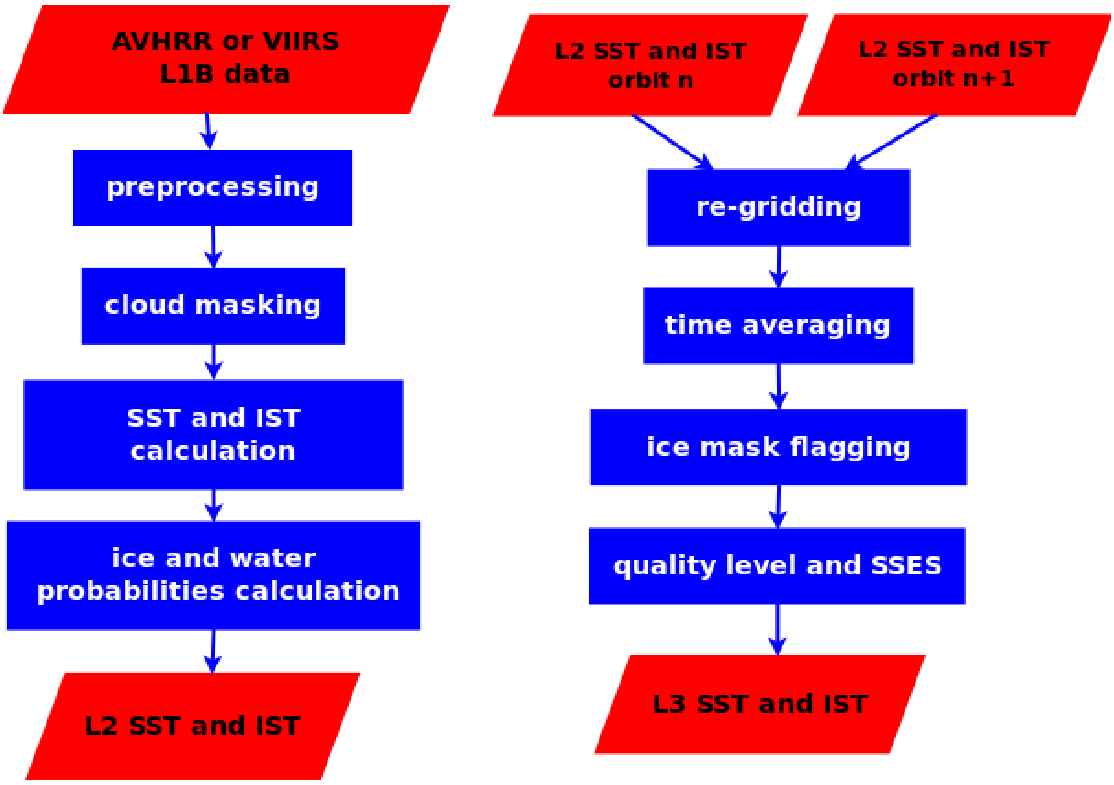

Figure 2: NHL OSI SAF Sea and Ice Surface Temperature L2 and L3 processing chains overview.

2.3 12-hourly L3 processing chain overview

The L3 12-hourly 5km HL SST/IST product is produced by combining available L2 satellite orbit SST/IST products, following the processing steps shown in Figure 2. The main components of the L3 processing are briefly described below.

2.3.1 Re-gridding

The re-gridding and time averaging is in a way done at the same time. The re-gridding first sets up the 5km polar stereographic NHL OSI SAF grid. All SST and IST observations/pixels from the different satellite passes are gridded to this grid by a nearest neighbour method (see 3.1 for details).

For each grid box the fraction of land is calculated from the land-sea information that is given in the satellite pass SST/IST file (taken from the land-sea atlas). If this fraction is larger than 50%, the grid box is marked as land.

In this gridding, the SST and IST pixels are treated separately, creating one SST field for all pure SST pixels, and one field for IST pixels. The IST field includes all pure ice pixels and marginal ice zone (MIZ) pixels.

In the gridding, the quality level of each pixel is also kept to be used during the time averaging. All pixels with quality level 2 and higher are used (see 3.3 for details).

2.3.2 Separation between open water and sea ice

Each L2 swath pixel is provided with a calculated probability for the pixel being cloud free open water and cloud free sea ice. These probabilities are used in an additional step (in addition to the PPS cloud mask classification) to further separate between open water and sea ice. See 3.2 for details.

2.3.3 Time averaging

The input to the 12-hourly product merging is all the available AVHRR satellite passes within the 12-hour period. The two daily 12-hourly products are centred at 00UTC and 12UTC, so that the 00UTC product covers all satellite passes from 18:00UTC the previous day to 05:59UTC the present day, and the 12UTC product covers 06:00 to 17:59UTC.

The averaging of SST/IST within each 5km grid box is done using the quality level of each observation (see 3.3 for details). Similarly to the SST/IST fields, a time field is calculated by averaging the times of all satellite pass SST/IST effectively used to calculate the final SST/IST value.

2.3.4 Additional sea ice flagging

There are two additional sea ice fields that are provided with the product. The first is a field containing a synthesis of the open water and sea ice probabilities provided in the L2 products used. More details are provided in 3.4.

The second is a field with a regridded version of the daily OSI SAF Sea Ice Edge product (OSI-402, see 2.4.1). The closest product in time is used (usually from the day before). This sea ice field is interpolated to the SST/IST 5km grid. All grid boxes that indicate sea ice in the Sea Ice Edge field (ice edge classes open ice and closed ice) are marked as sea ice in a separate sea ice field.

2.3.5 Quality level and SSES

As described in 2.3.3, the quality level of each grid box is determined in the time averaging. The error specification of this grid box then follows the quality level, as each quality level has its specific error estimates. These errors are called Sensor Specific Error Specification (SSES) and is further described in 4.3.

2.4 Auxiliary data

2.4.1 OSI SAF sea ice edge product

The OSI SAF sea ice edge product is used for providing an additional ice mask information in the OSI-203-b product. This sea ice edge product has three classes; open water, open sea ice and closed sea ice. The boarder between open water and open sea ice is at about 35% sea ice concentration. More details about the sea ice edge product user manual [RD.4].

2.4.2 Land-sea-mask

The land-sea-mask is based on the same mask as the OSI-205-b product, (NOAAngdc, 2014-09), see [RD.1] for details. This land-sea-mask has been gridded to the OSI-203-b grid. All grid boxes with less than 10% land is regarded as sea. Only L2 OSI-205-b pixels with 0% land are used in the OSI-203-b product.

2.5 Computer and programming considerations

The principles of gridding and averaging the OSI-205-b L2 input files to this L3 product are fairly simple, and this chain will not pose any major constrains associated with processing power, memory usage or data storage.

The OSI-203-b processing chain is written in Python 2.7 programming language using common libraries such as numpy, scipy, basemap and netcdf4.

The final NetCDF product file will have a size of about 50Mb, so a total daily volume of about 100Mb. The final GRIB product file will have less layers, and hence have less volume.

3 12-hourly L3 processing chain algorithms descriptions

The L2 processing described in [RD.1] provides all the SST and IST calculations including quality levels needed for the L3 processing. The few L3 processing algorithms are described below.

3.1 Re-gridding

The re-gridding of the L2 SST/IST swath data is done on a pixel-basis, so that each L2 swath observation with a valid SST or IST value is gridded to the L3 grid. This gridding is performed using the PROJ.4 Cartographic Projections library (available at http://proj.osgeo.org). Latitude and longitude values from the L2 swath are transformed to coordinate values in the 5km polar stereographic output grid. A nearest neighbour method is applied in the gridding.

3.2 Separation between open water and ice

The L2 product comes with probability of the pixel being cloudy (Pc), cloud free water (Pw) and cloud free sea ice (Pi), in addition to the PPS cloud mask. Actually, only Pw and Pi are provided, but Pc = 1 – Pi – Pw since this is a 3-way classifier. These probabilities are used for an additional quality check step, before the pixels are averaged in each product grid box.

The following steps are used for SST pixels:

1. If Pi > 0.90 or Pc > 0.90, the quality level is reduced by 2 levels.
2. Else if Pw < 0.95, the quality level is reduced by 1 level.
3. Then, if the quality level then is < 2, the pixel is marked as cloudy.

The following steps are used for IST pixels:

1. If Pw > 0.90 or Pc > 0.90, the quality level is reduced by 2 levels.
2. Else if Pi < Pw and Pc < 0.10, the quality level is reduced by 1 level.
3. Then, if the quality level then is < 2, the pixel is marked as cloudy.

The threshold of 0.9 (90% probability) in the test 1 both for SST and IST is used as a strong indication of the pixel not containing a valid SST or IST, and hence the quality level is reduced by 2 levels. Test 2 in the two cases is used as an indication that this pixel might not be completely cloud-free water (SST) or cloud-free ice (IST).

The quality levels are changed like this because the probabilities are not used in the calculation of the L2 quality levels.

If there are no probability estimates, the OSI SAF ice edge mask is used instead. For each output grid cell where the ice edge value is open ice or closed ice, and L2 indicates an SST value, this SST value is masked as ice.

The source of ice masking will be provided in the processing flag provided with the product, so that the user can see where it has been applied. In addition, the OSI SAF ice concentration field is included as a field in the product file.

3.3 Time averaging

The averaging within each 5km grid box is done using the quality level of each observation. The quality level from the L2 product is a value between 5 and 0, where 5 is the highest confidence and 2 is the lowest quality level with a valid SST/IST value (see [RD.1]). All the observations inside one grid box from the time averaging period are compared and only the observations with the highest available quality level are used. If one observation has a quality level higher than the rest, only that observation is used. The SST/IST value of the grid box is then the mean of all the observations with the highest quality level. This quality level is then assigned to this grid box. The number of observations contributing to each grid box is kept and provided in a separate field. In this way no observations with different quality level is mixed within one grid box.

The ice edge marks the border between open sea where SST is calculated and the marginal ice zone and closed ice where IST is calculated. This border changes during the 12 hour period of the time averaging. So, if the regridding provides both SST values and IST values in a grid box from the different L2 swath products, the grid box is considered partly ice covered and the average of the highest quality SST and IST values are used in the time averaging.

3.4 Calculation of average probability fields

A synthesis of the open water and sea ice probabilities provided with the L2 input product is calculated and provided with the SST/IST L3 product. This is done by calculating the average open water and sea ice probabilities within each L3 grid box, using all pixels where the probability of clouds is less than 10%. The average probability of sea ice is then provided with the L3 product.

4 Validation and Technical Aspects

4.1 Product control

The aim of the continuous control is to monitor the stability and quality of the product. This automatic control has a daily and a monthly part. The daily part consists in the calculation for each 12-hourly product of the rate of quality levels calculated as the percentage of pixels having a particular quality level with respect to the total number of pixels. The total geographical coverage of the product is also monitored. The purpose of this daily control is to check that the product behaves in a stable way on a day-to-day basis.
On a monthly basis the standard deviation and bias of estimated satellite SST/IST compared with observed in situ SST/IST are compared. For both the daily and monthly quality control warnings are issued to the production team if the values reaches certain threshold levels.

4.2 Algorithm validation

For the validation of the SST/IST product a matchup dataset (MDS) is built routinely collocating in situ measurements (buoys and ships) and satellite estimates of SST/IST for 12-hourly products. There are separate MDSs for SST and IST due to the different availability to in situ observations, but in the same file format.

For SST, the in situ data are collected through GTS from drifting buoys, moored buoys and ships, in addition to ship-board radiometer observations when available. These observations are quality controlled. Then the observations are collocated with the SST product and auxiliary information. For the MDS building the SST product data are collected in a 5x5 pixel box centered at the product pixel corresponding to the observation point. Only cloud free data are used and the cloud cover in the pixel box is calculated. The matchup time window is +/- 6 hours.

For IST, in situ data from drifting buoys on the ice surface are collected through GTS as for ST. These in situ observations are not the optimal source of validation data as the representativity of the observation for the sea ice skin temperature is questionable. The measure a combination of air/snow/ice temperature. So, in addition, the validation efforts also consist of collecting campaign data from in situ IR radiometer data over ice and snow.

From the matchup dataset various statistics are calculated to validate the accuracy and precision of the products, mainly by investigating the bias and standard deviation of the estimated SST compare to the in situ measurement. For all operational products these results are reported in the OSI SAF Half Yearly Operations Report and on the OSI SAF web site, all available at http://www.osi-saf.org.
The product is validated against the target accuracy value, as described in [RD.3], and shown in Figure 3.

Product ID	Product Name	Product Acronym	Product Type	Operational Satellite Input Data	Other Operational Input Data	Characteristics and Methods	Dissemination Means	Format	Production Frequency	End-to-end timeliness	Spatial Coverage	Spatial sampling	Threshold Accuracy	Target Accuracy	Optimal Accuracy	Verification/ Validation Methods
OSI-203-b	Northern High Latitude Sea and Sea Ice Surface Temperature	NHL SSIST	NRT Product	AVHRR (Metop) and VIIRS (NPP, JPSS)	ECMWF outputs	SST: subskin temperature. SIST: skin temperature. Multispectral algorithms.	FTP server, EUMETCast, data centre	NetCDF, GRIB	2 per day	3h30	Poleward of 50N	5 km	SST bias: 1°C SST std: 1,5°C SIST bias: 2.0 / 3.0°C SIST std: 3.0 / 4.0°C (1)	SST bias: 0.5°C SST std: 0.8°C SIST bias: 1.0 / 1.5°C SIST std: 1.5 / 2.0°C (1)	SST bias: 0.1°C SST std: 0.3°C SIST bias: 0.5 / 0.8°C SIST std: 0.8 / 1.0°C (1)	SST: Comparison with buoy observations. SIST: comp with IR radiometer and buoy obs, separately (1)

Figure 3: List of requirements for OSI-203-b, including target accuracy, from [RD.3].

4.3 Error estimates

Sensor Specific Error Estimates (SSES) will be provided for each pixel, based on the GHRSST common principles (GHRSST, 2012). The SSES are observational error estimates provided at pixel level as a bias and standard deviation. These SSES statistics will be based on the validation exercise to be performed during the implementation of the processing software, using one full year of data.

4.4 Exception handling

1. In the case of no L2 data available for parts (or all) of the L3 product area, no SST or IST values will be calculated, and a fill-value will be provided with appropriate processing flag.
2. In the case of the expected sea ice product file is missing, an older sea ice product file will be used.

4.5 Assumptions and Limitations

1. There may be periods where the statistical basis for IST validation is limited, due to varying number of available in in situ observations.
2. The error estimates presented in the SSES for each SST and IST estimates are average values and represent typical error values for the SST and IST retrieval.

5 References

GHRSST (2012): The recommended GHRSST Data Specification, GDS 2.0 revision 5. Available on https://www.ghrsst.org/documents.

McClain, E.P., W.G. Pichel and C.C. Walton (1985): Comparative performance of AVHRR-based multichannel sea surface temperatures. J. Geophys. Res., **90**, p.11587.

NOAAngdc. National Oceanic and Atmospheric Administration, National Geophysical Data Centre. http://www.ngdc.noaa.gov/mgg/global/global.html, 2014-09.

Walton C. C., W. G. Pichel, J. F. Sapper, D. A. May (1998): The development and operational application of nonlinear algorithms for the measurement of sea surface temperatures with the NOAA polar-orbiting environmental satellites, J. Geophys. Res., 103: (C12) 27999-28012.

6 Appendix A: Example of product header

The following is a draft example the L3 SST/IST NetCDF product header. Some details still needs to be confirmed.

```
dimensions:
        nj = 900 ;
        ni = 1260 ;
        time = 1 ;
variables:
        float lat(nj, ni) ;
                lat:standard_name = "latitude" ;
                lat:valid_min = -90.f ;
                lat:valid_max = 90.f ;
                lat:units = "degrees_north" ;
                lat:comment = "geographical coordinates, WGS84 projection" ;
        float lon(nj, ni) ;
                lon:standard_name = "longitude" ;
                lon:valid_min = -180.f ;
                lon:valid_max = 180.f ;
                lon:units = "degrees_east" ;
                lon:comment = "geographical coordinates, WGS84 projection" ;
        int Polar_Stereographic_Grid ;
                Polar_Stereographic_Grid:grid_mapping_name = "polar_stereographic" ;
                Polar_Stereographic_Grid:straight_vertical_longitude_from_pole = 0. ;
                Polar_Stereographic_Grid:latitude_of_projection_origin = 90. ;
                Polar_Stereographic_Grid:standard_parallel = 60. ;
                Polar_Stereographic_Grid:semi_major_axis = 6371000. ;
                Polar_Stereographic_Grid:semi_minor_axis = 6371000. ;
                Polar_Stereographic_Grid:proj4_string = "+proj=stere +a=6371000 +lon_0=0
+lat_ts=60 +b=6371000 +lat_0=90" ;
        short l2p_flags(time, nj, ni) ;
                l2p_flags:long_name = "L3C flags" ;
                l2p_flags:valid_min = 0s ;
                l2p_flags:valid_max = 255s ;
                l2p_flags:flag_meanings = "microwave land ice lake river
reserved_for_future_use no_retrieval validation" ;
```

```
		l2p_flags:flag_masks = 1s, 2s, 4s, 8s, 16s, 32s, 64s, 128s ;
		l2p_flags:comment = "These flags can be used to further filter data variables" ;
		l2p_flags:coordinates = "lon lat" ;
		l2p_flags:grid_mapping = "Polar_Stereographic_Grid" ;
	byte sses_bias(time, nj, ni) ;
		sses_bias:_FillValue = -128b ;
		sses_bias:long_name = "SSES bias error" ;
		sses_bias:units = "kelvin" ;
		sses_bias:valid_min = -127b ;
		sses_bias:valid_max = 127b ;
		sses_bias:add_offset = -0.64f ;
		sses_bias:scale_factor = 0.01f ;
		sses_bias:comment = "SSES bias error" ;
		sses_bias:coordinates = "lon lat" ;
		sses_bias:grid_mapping = "Polar_Stereographic_Grid" ;
	byte sses_standard_deviation(time, nj, ni) ;
		sses_standard_deviation:_FillValue = -128b ;
		sses_standard_deviation:long_name = "SSES standard deviation" ;
		sses_standard_deviation:units = "kelvin" ;
		sses_standard_deviation:valid_min = -127b ;
		sses_standard_deviation:valid_max = 127b ;
		sses_standard_deviation:add_offset = 0.f ;
		sses_standard_deviation:scale_factor = 0.01f ;
		sses_standard_deviation:comment = "SSES standard deviation" ;
		sses_standard_deviation:coordinates = "lon lat" ;
		sses_standard_deviation:grid_mapping = "Polar_Stereographic_Grid" ;
	int time(time) ;
		time:units = "seconds since 1981-01-01 00:00:00" ;
		time:long_name = "reference time" ;
		time:comment = "Includes leap seconds since 1981" ;
	short sst_dtime(time, nj, ni) ;
		sst_dtime:_FillValue = -32768s ;
		sst_dtime:long_name = "time difference from reference time" ;
		sst_dtime:units = "seconds" ;
		sst_dtime:add_offset = 0.f ;
```

sst_dtime:scale_factor = 60.f ;

sst_dtime:valid_min = -32767s ;

sst_dtime:valid_max = 32767s ;

sst_dtime:comment = "Variable time plus sst_dtime gives seconds after 00:00:00 UTC January 1, 1981" ;

sst_dtime:coordinates = "lon lat" ;

sst_dtime:grid_mapping = "Polar_Stereographic_Grid" ;

short sea_surface_temperature(time, nj, ni) ;

sea_surface_temperature:_FillValue = -32768s ;

sea_surface_temperature:units = "kelvin" ;

sea_surface_temperature:long_name = "sea surface subskin temperature" ;

sea_surface_temperature:standard_name = "sea_surface_subskin_temperature" ;

sea_surface_temperature:depth = "1.5 millimetres" ;

sea_surface_temperature:add_offset = 273.15f ;

sea_surface_temperature:scale_factor = 0.01f ;

sea_surface_temperature:valid_min = -200s ;

sea_surface_temperature:valid_max = 3000s ;

sea_surface_temperature:coordinates = "lon lat" ;

sea_surface_temperature:grid_mapping = "Polar_Stereographic_Grid" ;

short sea_ice_surface_temperature(time, nj, ni) ;

sea_ice_surface_temperature:_FillValue = -32768s ;

sea_ice_surface_temperature:units = "kelvin" ;

sea_ice_surface_temperature:long_name = "sea ice surface skin temperature" ;

sea_ice_surface_temperature:standard_name = "sea_surface_skin_temperature" ;

sea_ice_surface_temperature:add_offset = 273.15f ;

sea_ice_surface_temperature:scale_factor = 0.01f ;

sea_ice_surface_temperature:valid_min = -200s ;

sea_ice_surface_temperature:valid_max = 3000s ;

sea_ice_surface_temperature:coordinates = "lon lat" ;

sea_ice_surface_temperature:grid_mapping = "Polar_Stereographic_Grid" ;

// global attributes:

:product_version = 2.2 ;

:geospatial_lat_units = "km" ;

:geospatial_lon_units = "km" ;

:references = "http://osisaf.met.no/docs/" ;

:platform = "MetOpA, NPP" ;

:Metadata_Conventions = "Unidata Observation Dataset v1.0" ;

:keywords = "Oceans > Ocean Temperature > Sea Surface Temperature" ;

:Conventions = "CF-1.4" ;

:id = "OSI-203-b" ;

:spatial_resolution = "5km" ;

:acknowledgment = "Please acknowledge the use of these data with the following statement: copyright (year) EUMETSAT." ;

:title = "EUMETSAT OSI SAF NHL Sea and Sea Ice Surface Temperature" ;

:standard_name_vocabulary = "NetCDF Climate and Forecast (CF) Metadata Convention" ;

:netcdf_version_id = 4.1 ;

:source = "AVHRR, VIIRS" ;

:sensor = "AVHRR, VIIRS" ;

:processing_level = "L3C" ;

:gds_version_id = 2.0r5 ;

:keywords_vocabulary = "NASA Global Change Master Directory (GCMD) Science Keywords" ;

:geospatial_lat_resolution = 5 ;

:metadata_link = "To be defined" ;

:creator_email = "osisaf-manager@met.no" ;

:institution = "EUMETSAT OSISAF" ;

:geospatial_lon_resolution = 5 ;

:creator_name = "OSISAF" ;

:creator_url = " http://osisaf.met.no" ;

:date_created = "20150323T193212Z" ;

:start_time = "20150323T064300Z" ;

:time_coverage_start = "20150323T064300Z" ;

:end_time = "20150323T170900Z" ;

:time_coverage_end = "20150323T170900Z" ;

:westernmost_longitude = TBD ;

:easternmost_longitude = TBD ;

:southernmost_latitude = TBD ;

:northernmost_latitude = TBD;